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Theoretical and Computational Approach to Modelling Flame Ignition

ELAINE S. ORAN AND JAY P. BORIS
Laboratory for Computational Physics

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20. Abstract (Continued)

of temperature can be used to calculate whether or not a given energy source is adequate to ignite the system. This simple procedure may then be calibrated using the time-dependent NRL detailed reactive flow models. The models include the thermophysical properties of the mixture, a full chemical kinetics scheme, the nonlinear convection of self-consistent fluid dynamics and the matrix molecular diffusion coefficients for the individual species. Results are presented for a selected mixture of $H_2-O_2-N_2$ for two values of R_0 which show that a model must be constructed for a quench volume in order to complete the similarity solution calibration.

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THEORETICAL AND COMPUTATIONAL APPROACH TO MODELLING FLAME IGNITION

Introduction

Ignition of fuel-oxidizer mixtures occur when an external source of energy initiates interactions among the controlling convective, transport and chemical processes. Whether the process results in deflagration, detonation, or is simply quenched depends on the intensity, duration, and volume affected by an external heat source. Ignition also will depend on the initial ambient properties of the mixture which determine the chemical induction time and the heat release per gram of material. This ignition is a complicated phenomena whose occurrence for a specific mixture of fuel and oxidizer depends strongly on diffusive and chemical parameters which are often very poorly known. A convenient, inexpensive way to estimate whether a mixture will ignite given a heat source intensity, duration, and volume would be both a valuable laboratory tool and a useful learning device.

This paper represents a summary of the work to date on the theoretical and computational effort at the Naval Research Laboratory in the study of the ignition of homogeneous gas phase mixtures. First the essential properties of a detailed, time-dependent, numerical model are presented. Then a description is given of a closed form similarity solution for the nonlinear time-dependent slow flow equations which forms the basis for a simple, time-dependent "hand-calculator" model of localized ignition. The similarity model requires minimal chemical and physical input and contains two constants which must be calibrated: the radii, or fraction of the time-dependent similarity solution radius, at which the thermal conductivity and induction parameters are evaluated. Finally, comparisons between two models are described for ignition of an $H_2-O_2-N_2$ mixture. The composition of the

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material and the length of time of energy deposition are held constant but the total energy deposition and the radius of deposition are allowed to vary.

The Detailed Simulation Model

In this section we describe the detailed numerical flame model and present a sample of calculations performed with it. The model permits a wide variety of geometric, initial, boundary and time-varying energy input conditions and was specifically developed to study the various physical and chemical processes which control flame initiation and quenching. Whereas propagation of a laminar flame has been successfully treated by steady state models, the details of initiation and quenching are inherently time-dependent phenomena and require detailed time-dependent models.

The model we have developed solves in one dimension the full set coupled conservation equations for total mass ρ , momentum ρv , and energy E as well as the individual species densities $\{n_j\}$:

$$\frac{\partial \rho}{\partial t} = - \nabla \cdot \rho v \quad (1)$$

$$\frac{\partial n_j}{\partial t} = - \nabla \cdot n_j v - \nabla \cdot n_j v + P_j - Q_j n_j \quad (2)$$

$$\frac{\partial \rho v}{\partial t} = - \nabla \cdot (\rho v v) - \nabla P + \nabla \cdot \eta_m (\nabla v + (\nabla v)^T) \quad (3)$$

$$\frac{\partial E}{\partial t} = - \nabla \cdot E v - \nabla \cdot (P v - \lambda \nabla T - Q_D) \quad (4)$$

The quantity \underline{v} is the fluid velocity, the $\{V_j\}$ are the diffusion velocities, and $\{P_j\}$ and $\{Q_j\}$ refer to the chemical production and loss processes for the individual species j . The quantities η_m and λ_m are the mixture viscosities or thermal conductivities using the expressions of Wilke (1950) and Mason and Saxena, (1958). The superscript "T" in the last term of Eq. (3) indicates that the transpose is to be taken. The quantity Q_D represents the contributions to the thermal conductivity due to diffusion processes and it is a function of $\{V_j\}$, the binary molecular diffusion coefficients $\{D_{jk}\}$, the thermal diffusion coefficients $\{D_j^T\}$, and the enthalpies $\{h_j\}$. Solution of the diffusion velocities includes the binary and thermal diffusion terms as well as the pressure gradient term, which in this flame is negligible. We also assume here that we are dealing with mixtures of ideal gases so that the pressure, P , may be written $P = Nk_B T$ where N is the total number density, k_B is Boltzmann's constant and T is the temperature. The model, however, is not restricted to ideal gases and in fact any equation of state may be used. Finally, we assume that there are no radiative losses in the system.

The technique for solving Eqs (1) - (4) is based on the method of asymptotic timestep splitting. The individual chemical and physical processes are integrated separately by the fastest and most accurate algorithms and then asymptotically coupled together. Advantages of this procedure over the more standard global implicit approaches (e.g. Westbrook, 1978; Lund, 1978) include faster calculations for modest and large numbers of species and more flexibility in problem configuration. The work presented here shows quite convincingly that our asymptotic coupling methods work accurately, reliably, and efficiently despite mistaken grumbling to the contrary.

The convective transport is solved by the algorithm ADINC (Boris, 1979), an implicit Lagrangian hydrodynamics algorithm for subsonic flows. The method allows for an arbitrary equation of state and gives an accurate representation of material interfaces. Thus it is also well suited to the analysis of heterogeneous combustion. ADINC communicates compression and expansion accross the system implicitly and yet maintains the steep gradients in species and temperature required for combustion modelling. The implicit pressure calculation overcomes the Courant timestep limit. Tests of the full detailed flame model in the limit of no chemical reactions of diffusive transport are essentially tests of the ADINC algorithm. A number of such tests have been documented in Boris, 1979. We further note that this algorithm lends itself to an adaptive gridding method in which cells are inserted or deleted according to externally specified physical conditions in the flow.

The chemical interactions are described by a set of nonlinear coupled ordinary differential equations. For this ignition calibration, we have used the H_2-O_2 reaction scheme given in Table I which involves the eight reactive species, H_2 , O_2 , O , H , OH , HO_2 , H_2O_2 , H_2O , and diluent which is chosen to be N_2 . The thermochemical properties of these species were taken from the JANAF tables (Stull and Prophet, 1971).

The final chemical rate scheme was arrived at after an extensive study of the literature especially aimed at updating the work of Baulch (1972). The mechanism was then tested extensively using the integration method VSAIM, which is a fully vectorized version of the selected asymptotic integration method, CHEMEQ, developed by Young (1977,1979). Many of these tests were performed in the limit of no convective or diffusive transport, which allowed detailed comparisons with measured induction times over a wide range of temperatures, pressures, and stoichiometries.

Typical results obtained by Burks and Oran (1980) are shown in Fig (1), which shows that we have obtained good agreement without any reaction rate adjustments. Thus we have confidence in both the reaction scheme and the integration method.

A new method has been devised to solve the $\{V_j\}$ accurately and without matrix inversion (Boris and Oran, 1978). The diffusion equations may be written

$$S_j = \sum_{\substack{k=1 \\ k \neq j}}^M \frac{n_j n_k}{N^2 D_{jk}} (V_k - V_j) \equiv \sum_{k=1}^M w_{jk} (V_k - V_j) \quad (5)$$

Where the source term S_j is defined by

$$S_j \equiv \nabla (n_j/N) - (\rho_j/\rho - n_j/N) \frac{\nabla P}{P} - \sum_{k=1}^M \frac{n_j n_k}{N^2 D_{jk}} (D_k^T/\rho_k - D_j^T/\rho_j) \frac{\nabla T}{T} \quad (6)$$

subject to the conditions,

$$\sum_{j=1}^M S_j = 0, \quad \text{and} \quad \sum_{j=1}^M \rho_j V_j = 0. \quad (7,8)$$

Then it may be shown that V_j may be written

$$V_j = \frac{-(\rho - \rho_j)}{\rho} \frac{N^2 D_{j\infty}}{(N - n_j) n_j} \left[\delta_{jk} + A_{jk} + A_{jl} A_{lk} + \dots \right] S_k \quad (9)$$

The $D_{j\Sigma}$, the diffusion coefficient of species j through the background provided by the sum of all the other species, is defined by

$$\frac{D_{j\Sigma}}{(N-n_j)} \sum_{k \neq j} \frac{n_k}{D_{jk}} \equiv 1 \quad (10)$$

and the matrix elements of A are given by

$$A_{jk} \equiv \frac{\rho_j}{\rho} \delta_{jk} + \frac{n_j}{D_{jk}} \frac{(\rho - \rho_k)}{\rho} \frac{D_{k\Sigma}}{(N-n_k)} (1 - \delta_{jk}) .$$

This algorithm is of $O(M^2)$ and is vectorized. Thus it is substantially faster than $O(M^3)$ matrix inversions when more than four of five species are involved.

The detailed model described above is currently written in ANSI standard Fortran and vectorized for operation in the Texas Instruments Advanced Scientific Computer. Running time is between .05 and .08 seconds for a timestep which includes evaluations of the full set of Eqs. (1) - (11) for 45 cells.

Results from a typical flame calculation in cartesian geometry are shown in Figs (2), (3) and (4). Figure (2) shows a typical temperature profile for a flame initiated by a quadratic temperature distribution at the onset of the calculation. Also shown on the same figure is a graph of the cell size, Δx , which shows that the resolution decreases as the absolute magnitude of temperature gradient increases. Species profiles are shown in Fig. (3) and details of the flame front in Fig (4). We note that the intermediate species and the temperature

gradients do not all peak at the same location and the structure of the flamefront is clearly distinguishable. This will be discussed more thoroughly in a future paper.

The Similarity Solution Model

The basic similarity solution is derived from the slow flow (Jones and Boris, 1977, Boris and Oran, 1978) approximation and is predicated on the assumption that energy addition to the system is slow enough that no appreciable energy is deposited in the heated region by shocks. Thus the system is characterized by (1) flow velocities which are small compared to the speed of sound, and (2) an essentially constant pressure field. The energy and velocity equations may then be written as

$$\frac{dP}{dt} \approx 0 = -\gamma P \nabla \cdot \underline{v} + \nabla \cdot \gamma N k_B \kappa \Delta T + S(t) e^{-k^2(t)r^2} \quad (12)$$

We also require the continuity equation which is written in the form

$$\frac{1}{\rho} \frac{d\rho}{dt} = -\nabla \cdot \underline{v} \quad (13)$$

In Eq. (12), γ is the ratio of heat capacities C_p/C_v , assumed here to be constant, and κ is a function of the mixture thermal conductivity, λ_m ,

$$\kappa \equiv \frac{\gamma-1}{\gamma N k_B} \lambda_m(T) \quad (14)$$

The last term on the right hand side of Eq. (12) is the source term. Proper choice of $S(t)$ ensures that a given amount of energy, E_0 , is deposited in a certain volume, $\frac{4\pi}{3} R_0^3$, in a time, τ_0 . It is the choice of this Gaussian profile which allows us to obtain a "closed" form similarity solution given below in spherical coordinates.

Using the assumption that $dP/dt \approx 0$, an algebraic equation is written for $\nabla \cdot \underline{v}$ from Eq. (12) which when combined with Eq. (13) gives

$$\frac{1}{T} \frac{dT}{dt} = \frac{S(t)}{P_\infty} e^{-k^2(t)r^2} + \frac{\nabla \cdot \underline{v}}{T} \quad (15)$$

where P_∞ is the background pressure. The solution is then

$$T(r,t) = T_\infty e^{A(t) e^{-k^2(t)r^2}} \quad (16)$$

$$\text{and } \rho(r,t) = \rho_\infty e^{-A(t) e^{-k^2(t)r^2}} \quad (17)$$

where T_∞ and ρ_∞ are the background temperature and pressure, respectively. Thus the nonlinear slow-flow equations including expansions and contractions of the flow have been converted into a single equation which is linear in the logarithm of the temperature.

The total energy of the system at any instant is the sum of the internal energy and the work performed in expanding the heated region. It may be written

$$E(t) = \frac{E_\infty \gamma}{\gamma - 1} \int_0^\infty 4\pi r^2 dr \left[1 - \frac{\rho(r,t)}{\rho_\infty} \right] \quad (18)$$

$$\begin{aligned}
&= \frac{\gamma \rho_{\infty}}{(\gamma-1) k^3(t)} \int_0^{\infty} 4\pi x^2 \left[1 - e^{-Ae^{-x^2}} \right] dx \\
&\equiv \frac{\gamma \rho_{\infty}}{(\gamma-1) k^3(t)} F(A(t))
\end{aligned} \tag{19}$$

which defines the intergral $F(A(t))$. Differentiating this we find that

$$\frac{dE}{dt} = \frac{\pi^{3/2} S(t)}{(\gamma-1) k^3(t)} \tag{20}$$

which may be equated to

$$\frac{dE}{dt} = \frac{\partial E}{\partial k} \frac{\partial k}{\partial t} + \frac{\partial E}{\partial A} \frac{\partial A}{\partial t} . \tag{21}$$

Thus a consistency condition has been specified on the rates of change of the amplitude, $A(t)$, and the scale size $k^{-1}(t)$ for the heated region.

If the fluid velocity v is then expanded such that

$$v(r) \approx v_1(t) r , \tag{22}$$

that is, only the linear term is kept, two coupled ordinary differntial equations for k and A may be obtained from Eqs. (15)- (21),

$$\frac{dk}{dt} = -kv_1 - 2\kappa k^3 \tag{23}$$

$$\frac{dA}{dt} = \frac{S(t)}{\gamma P} - 6\kappa k^2 A \tag{24}$$

and we also find that

$$v_1 = \frac{S}{3\gamma P_\infty} \frac{F'(0) - F'(A)}{F(A)} + 2\kappa k_B^2 \frac{AF'(A) - F(A)}{F(A)}. \quad (25)$$

This last expression for v_1 , Eq. (25) is basically the result of invoking energy conservation through equating Eqs. (20) and (21) and is the first calibration in the model.

The model requires one further definition in order to predict ignition. A curve of chemical induction time as a function of temperature must be included in order to define the induction parameter,

$$I(t) = \int_0^t \frac{dt'}{\tau_c(T(r,t'))}. \quad (26)$$

Ignition "occurs" when $I(t) = 1$ in this model, which is an exact result in the limit of large heat source and constant temperature near the center of the heated region. A simple analytic expression for $\tau_c(T)$ depending on three constants has been derived and can be calibrated using as few as three distinct values of τ_c at different temperatures. These values may be obtained from detailed kinetic calculations, a few measured points in the curve, or from educated guesses.

Model Comparisons

In order to compare the results from the detailed simulation model to that of the similarity model, the detailed model has been configured for spherical symmetry with open boundary conditions. Energy is then deposited in a Gaussian profile with a characteristic radius which closely matches the one derived from the similarity model. Energy deposition in both models is assumed linear in time at a rate determined by requiring an energy E_0 to be deposited in a time τ_0 . Note that the characteristic radius for energy deposition, R_c , increases with time.

The chemical model for these first tests was taken to be a mixture of $H_2:O_2:N_2$ in the ratios 2:1:10 at 1 atm and $T_{\infty}=300^{\circ}K$. The curve of the induction time as a function of temperature for this mixture is shown in Fig. (5) and was derived from the detailed studies of the H_2-O_2 mechanisms (Burks and Oran, 1980).

In the similarity model, κ was estimated by comparing the formula at $300^{\circ}K$,

$$\lambda_M^S = \frac{8.2 \times 10^3}{\bar{\sigma}^2} \sqrt{\frac{T(^{\circ}K)}{\bar{M}}} \frac{\text{erg}}{\text{cm sec } ^{\circ}K}, \quad (27)$$

which assumes that an average molecular distance $\bar{\sigma}$ and an average molecular weight \bar{M} may be found, to the more exact formulation

$$\lambda_M = \left[\lambda_j \left[1 + \frac{1}{2\sqrt{2}} \sum_{k \neq j} n_k w_{jk} \right] \right]^{-1}$$

where W_{jk} is a function of $\{\lambda_j\}$ and the atomic masses $\{m_j\}$ suggested by Mason and Saxena. This gives us

$$\bar{\sigma} = 3.16 \text{ A}$$

$$\bar{M} = 24.3.$$

This approximation is valid because the similarity solution is only accurate for ignition before any major amount of product or intermediates are formed. Then the parameter κ is found using the definition in Eq (4). Determining the temperature (radius) at which κ is to be evaluated is part of the calibration to be done.

In the first case studies,

$$R_0 = .1 \text{ cm}$$

$$\tau_0 = 1.0 \times 10^{-4} \text{ sec.}$$

By varying E_0 , the similarity solution indicates that the minimum ignition energy is about 3.3×10^4 ergs. Figs. (6a and b) show the typical behavior of $A(t)$, $R_c(t)$, $T(R=0)$ and $I(t)$ for 3.3×10^4 ergs. The functions $I(t)$ and $\kappa(t)$ were evaluated at the central temperature, $R=0.0\text{cm}$, although calculations in which these quantities were evaluated at $R=R_c$ were virtually indistinguishable. Results from the corresponding detailed simulations are shown in Fig (7) for three values of E_0 . A comparison then tells us that agreement between the similarity solution and the detailed simulation is good. We note here that for this case both models predict ignition at essentially the same time for a range of input energies.

In the second example,

$$R_0 = 0.025 \text{ cm}$$

$$\tau_0 = 1 \times 10^{-4} \text{ sec.}$$

The similarity model predicts a minimum ignition energy of $\sim 8 \times 10^2$ ergs. However, for the range of energies tested, up to 1×10^4 ergs, the full simulation does not show ignition, but predicts that some burning does occur and the flame is eventually quenched. Note however that although flame propagation is not predicted in these simulations, the values of $I(t)$ and $\kappa(t)$ were evaluated at the central temperature. Evaluating them at a further radius, $R=R_c$, did not improve agreement. The similarity model must be calibrated by evaluating both $\kappa(t)$ and $I(t)$ at a particular characteristic radius which in this case must be even larger than $R=R_c$.

Conclusion

We have thus shown the existence of a quench volume which has been discussed previously in the literature by, for example, Lewis and von Elbe (1961), Dixon-Lewis (1978) and Overley et al (1978). It occurs in the simulation mentioned above because of the relatively swift effects of molecular diffusion in the small volume in which the energy is deposited. We know that for a particular geometry and gas mixture, the quench volume must be related to R_0 , τ_0 , E_0 and the properties of the material $\lambda_m(T)$, $\{h_j(t)\}$, γ , and τ_c . We are currently using the combination of the similarity and detailed simulations to test various approximations for the quenching volume and to test the sensitivity of this volume to the manner in which chemical reaction is initiated.

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CHEMICAL REACTION RATES

Reaction Rate Constants*

$$k = AT^B e^{C/T}$$

	Reactants	Products	A	B	C	Reference†
1.	H + H + M	H ₂ + M	1.80(-30)	-1.00	0.00	Baulch et al., 1972
2.	H + O + M	OH + M	8.28(-29)	-1.00	0.00	Bahn, 1969
3.	H + OH	H ₂ + O	1.40(-14)	1.00	-3.50(+03)	Baulch et al. 1972
4.	H + OH + M	H ₂ O + M	6.20(-26)	-2.00	0.00	Baulch et al., 1972
5.	H + H ₂ O	H ₂ + OH	1.79(-14)	1.20	-9.61(+03)	Cohen and Westberg, 1978
6.	H + O ₂	O + OH	3.70(-10)	0.00	-8.45(+03)	Baulch et al., 1972
7.	H + O ₂ + M	HO ₂ + M	4.10(-35)	0.00	5.00(+02)	Baulch et al., 1972
8.	H + HO ₂	H ₂ + O ₂	4.20(-11)	0.00	-3.50(+02)	Baluch et al., 1972
9.	H + HO ₂	O + H ₂ O	8.30(-11)	0.00	-5.00(+02)	Hampson, 1975
10.	H + HO ₂	OH + OH	4.20(-10)	0.00	-9.50(+02)	Baulch et al., 1972
11.	H + H ₂ O ₂	H ₂ + HO ₂	2.80(-12)	0.00	-1.90(+03)	Baulch et al., 1972
12.	H + H ₂ O ₂	HO + H ₂ O	5.28(-10)	0.00	-4.50(+03)	Baulch et al., 1972
13.	H ₂ + O	H + OH	3.00(-14)	1.00	-4.48(+03)	Baulch et al., 1972
14.	H ₂ + OH	H + H ₂ O	1.83(-15)	1.30	-1.84(+03)	Cohen and Westberg, 1978
15.	H ₂ + O ₂	H + HO ₂	9.10(-11)	0.00	-2.91(+04)	Baulch et al., 1972
16.	H ₂ + O ₂	OH + OH	2.80(-11)	0.00	-2.42(+04)	Olson, 1977
17.	H ₂ + HO ₂	H + H ₂ O ₂	1.20(-12)	0.00	-9.40(+03)	Baulch et al., 1972
18.	H ₂ + HO ₂	OH + H ₂ O	1.21(-12)	0.00	-9.41(+03)	Olson, 1977
19.	H ₂ + M	H + H + M	3.70(-10)	0.00	-4.83(+04)	Baulch et al., 1972
20.	O + O + M	O ₂ + M	5.00(-35)	0.00	9.00(+02)	Baulch et al., 1972
21.	O + OH	H + O ₂	2.72(-12)	2.80(-01)	8.10(+01)	k _f = k _r K _C
22.	O + OH + M	HO ₂ + M	2.80(-31)	0.00	0.00	Bahn, 1969

Reaction Rate Constants

$$k \approx AT^B e^{C/T}$$

	Reactants	Products	A	B	C	Reference
23.	O + H ₂ O	H + HO ₂	1.75(-12)	4.50(-01)	-2.84(+04)	k _r = k _f /K _c
24.	O + H ₂ O	OH + OH	3.20(-15)	1.16	-8.77(+03)	k _r = k _f /K _c
25.	O + HO ₂	OH + O ₂	8.30(-11)	0.00	-5.03(+02)	Lloyd, 1974
26.	O + H ₂ O ₂	OH + HO ₂	1.40(-12)	0.00	-2.13(+03)	Hampson, 1975
27.	O + H ₂ O ₂	O ₂ + H ₂ O	1.4(-12)	0.00	-2.12(+03)	Hampson, 1975
28.	OH + OH	H + HO ₂	2.00(-11)	0.00	-2.02(+04)	Baulch, et al, 1972
29.	OH + OH	H ₂ + O ₂	1.09.(-13)	2.60(-01)	-1.47(+04)	k _f =k _r K _c
30.	OH + OH	O + H ₂ O	1.00(-16)	1.30	0.00	Cohen & Westberg, 1978
31.	OH + OH + M	H ₂ O ₂ + M	2.50(-33)	0.00	2.55(+03)	Baulch, et al, 1972
32.	OH + HO ₂	H ₂ O + O ₂	8.30(-11)	0.00	-5.00(+02)	Lloyd, 1974
33.	OH + HO ₂	O + H ₂ O ₂	2.07(-15)	6.4(-01)	-8.23(+03)	k _r = k _f /K _c
34.	OH + H ₂ O	H ₂ + HO ₂	1.34(-14)	4.30(-01)	-3.62(+04)	k _f = k _r K _c
35.	OH + H ₂ O	H + H ₂ O ₂	2.99(-10)	0.00	-4.05(+04)	k _r = k _f /K _c
36.	OH + O ₂	HO ₂ + O	2.20(011)	1.80(-01)	-2.82(+04)	k _r = k _f /K _c
37.	OH + H ₂ O ₂	H ₂ O + HO ₂	1.70(-11)	0.00	-9.10(+02)	Baulch, et al., 1972
38.	OH + M	H + O + M	2.33(-10)	2.10(-01)	-5.10(+04)	k _r = k _f /K _c
39.	H ₂ O + O ₂	OH + HO	2.38(-10)	1.70(-01)	-3.69(+04)	k _r = k _f /K _c

Reaction Rate Constants

$$k = AT^B e^{C/T}$$

	Reactants	Products	A	B	C	Reference
40.	H ₂ O + HO ₂	OH + H ₂ O ₂	4.70(-11)	0.00	-1.65(+04)	Baulch, et al., 1972
41.	H ₂ O + M	H + OH + M	5.80(-09)	0.00	-5.29(+04)	Baulch, et al., 1972
42.	O ₂ + H ₂ O ₂	HO ₂ + HO ₂	1.57(-09)	-3.77(-01)	-2.20(+04)	k _r = k _f /K _C
43.	O ₂ + H ₂ O ₂	O + H ₂ O ₂	5.70(-14)	5.20(-1)	-4.48(+04)	k _r = k _f /K _C
44.	O ₂ + M	O +) + M	3.00(-06)	-1.00	-5.94(+04)	Baulch, et al., 1972
45.	HO ₂ + HO ₂	O ₂ + H ₂ O ₂	3.00(-11)	0.00	-5.00(+02)	Hampson, 1975
46.	HO ₂ + M	H + O ₂ + M	3.50(-09)	0.00	-2.30(+04)	Baulch, et al., 1972
47.	HO ₂ + M	O + OH + M	1.13(-04)	-4.30(-01)	-3.22(+04)	k _r = k _f /K _C
48.	H ₂ O ₂ + M	OH + OH + M	2.00(-07)	0.00	-2.29(+04)	Baulch, et al., 1972

*Bimolecular Rate Constants are given in units of cm³/molecule sec, T in °K.

Termolecular Rate Constants are in cm⁶/molecular sec where M is the third body.

**Read 1.80(-30) as 1.80 x 10⁻³⁰.

†K_C computed based on data in Janaf tables.

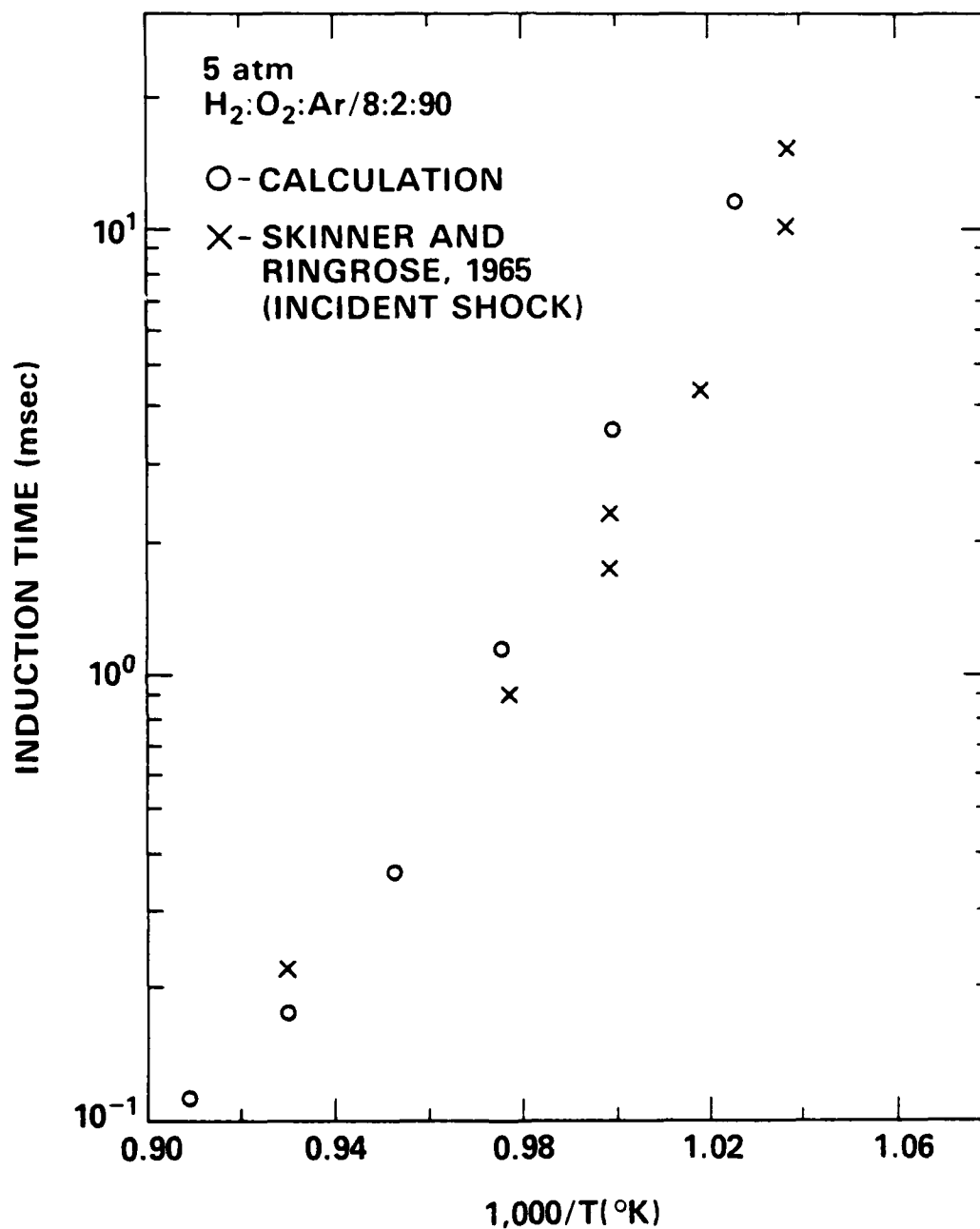


Fig. 1 - Comparisons between induction times calculated using the $\text{H}_2\text{-O}_2$ reaction scheme in Table I and the measurements of Skinner and Ringrose, 1965

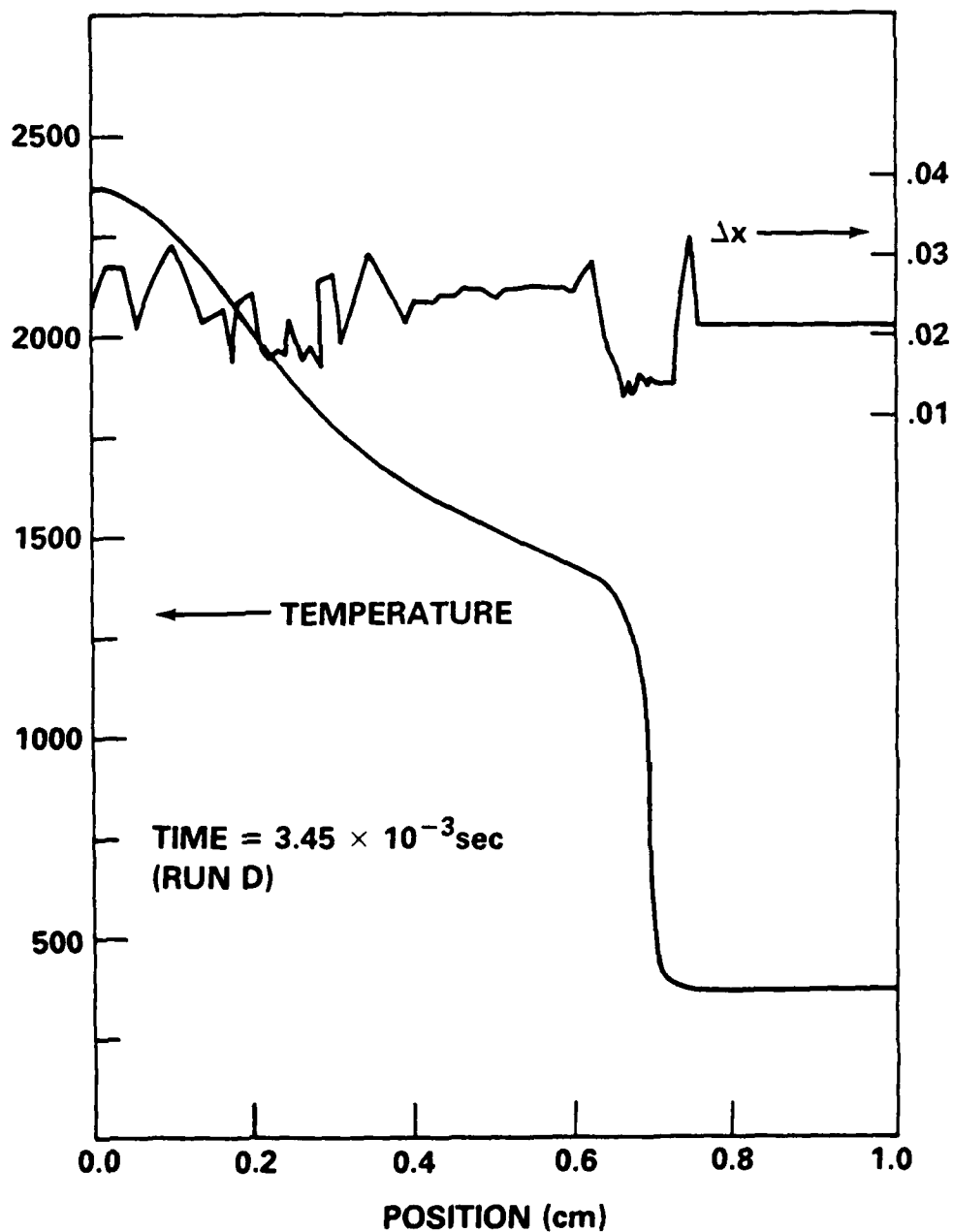


Fig. 2 - Temperature profile calculated from the detailed simulation model for a flame in an $H_2:O_2:N_2/2:1:10$ mixture ignited by a quadratic temperature profile at the onset of the calculation. Also shown is a graph of the cell size, x , as a function of position.

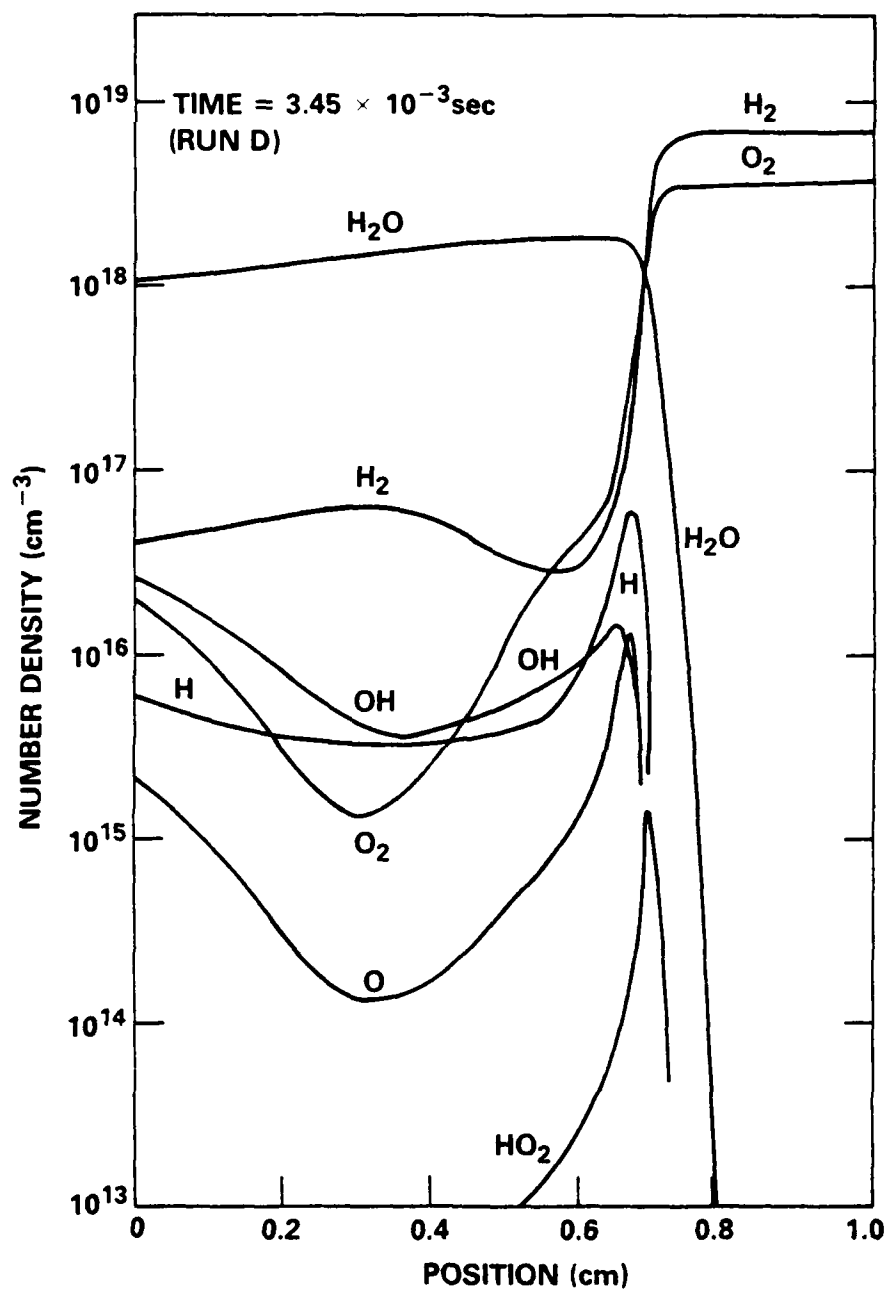


Fig. 3 - Calculated profiles of species concentrations corresponding to the temperature profile in Fig. 2.

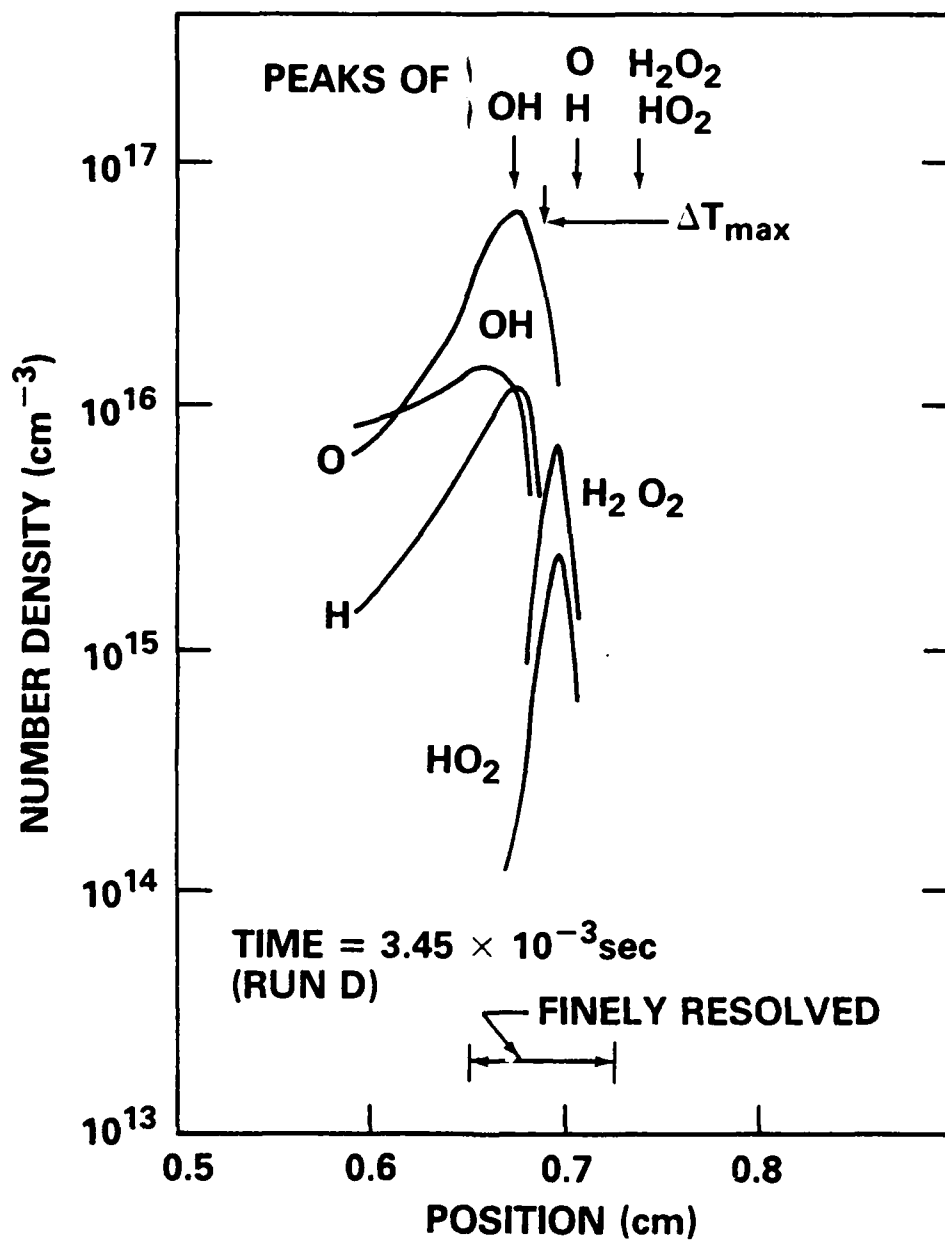


Fig. 4 - Calculated profiles of intermediate species concentrations at the flame front corresponding to Figs. 2 and 3. The fine resolution around the flame front allows differentiation of the peak densities of the intermediate species.

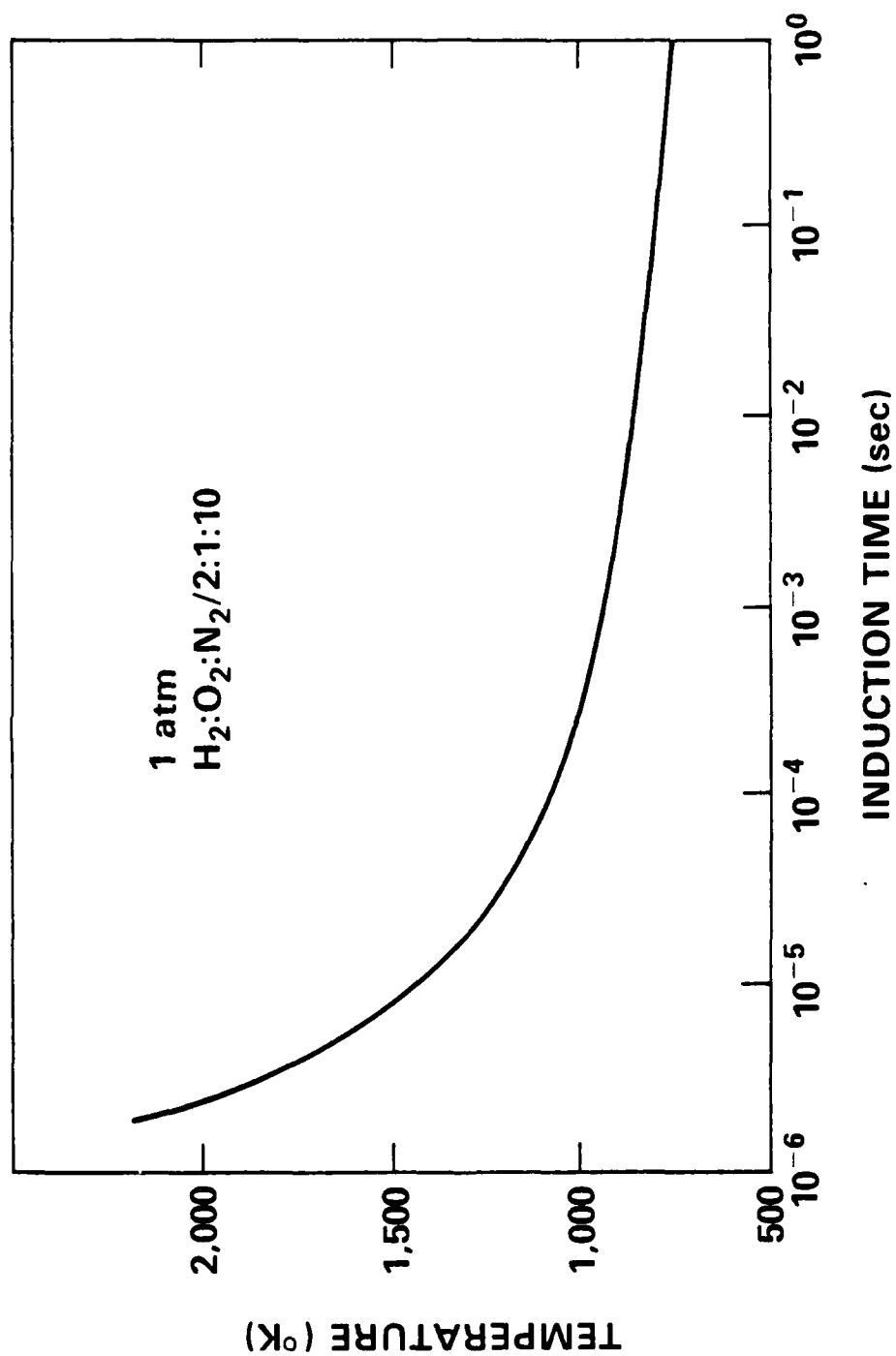


Fig. 5 - Temperature as a function of induction time for a mixture of $H_2:O_2:N_2/2:1:10$ calculated using the reaction scheme in Table I.

$T_0 = 1.0 \times 10^{-4}$ sec. $E_0 = 3.3 \times 10^4$ ergs. $R_0 = 0.1$ cm

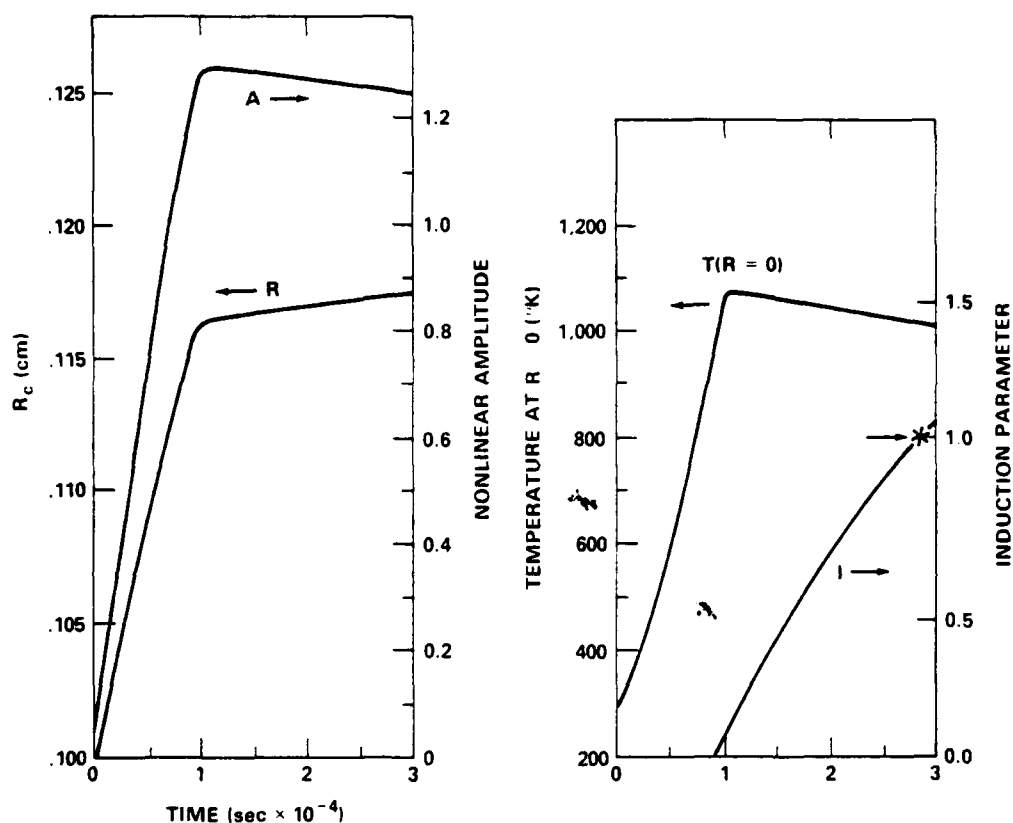


Fig. 6 - The amplitude, A , the characteristic radius, R , the central temperature, $T(R=0)$, and the induction parameter, I , as a function of time calculated with the similarity solution model for input energy, $E_0 = 3.3 \times 10^4$, in a volume of radius, $R_0 = 0.1$ cm, in a time, $T_0 = 1 \times 10^{-4}$ sec. The "*" indicates the predicted time of ignition.

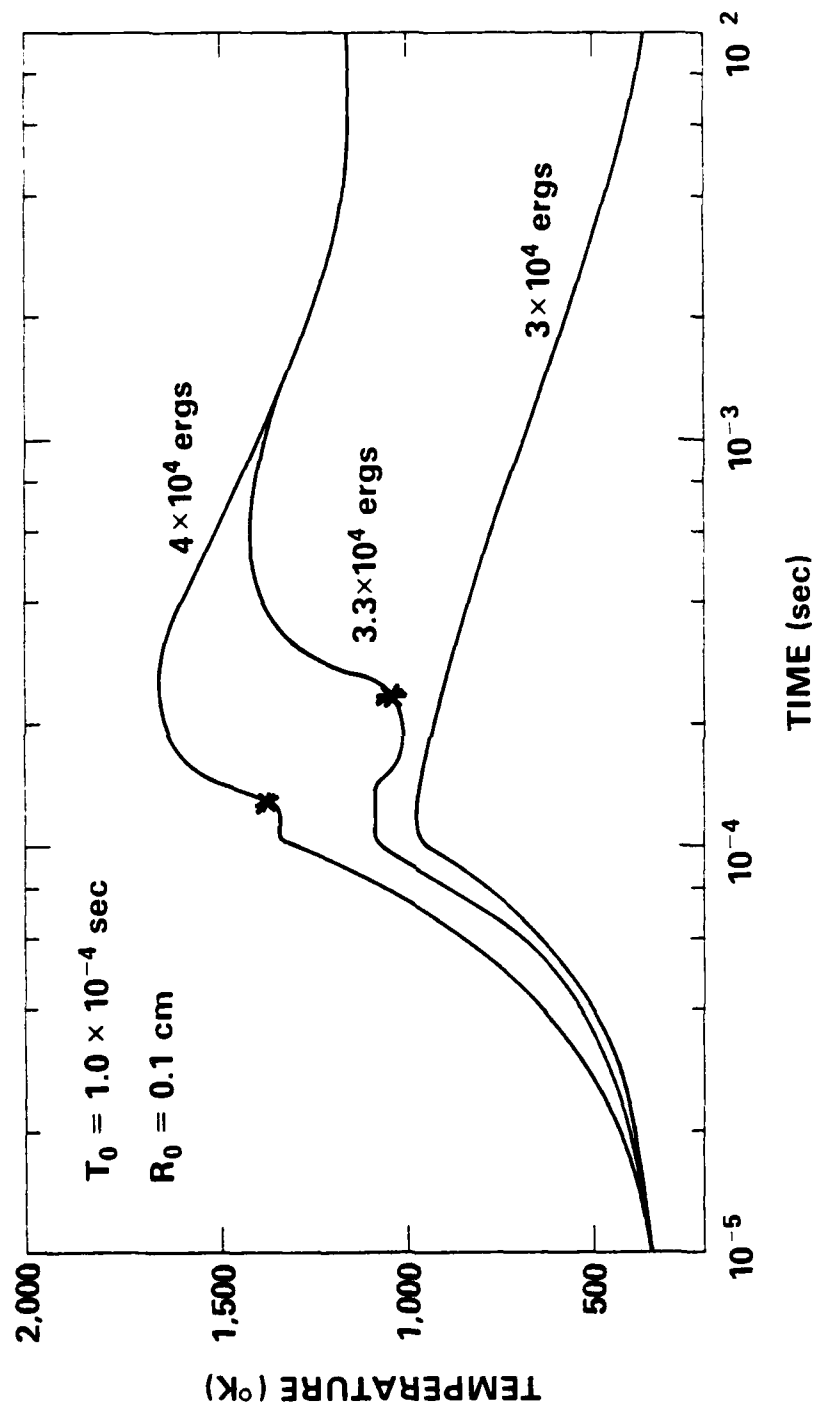


Fig. 7 - Calculations of the central temperature as a function of time for $T_0 = 1 \times 10^{-4} \text{ sec}$, $R_0 = 0.1 \text{ cm}$, and varying E_0 using the detailed simulation model. The ignition times agree well with those predicted by the similarity solution.